Bias-Variance and Cross Validation

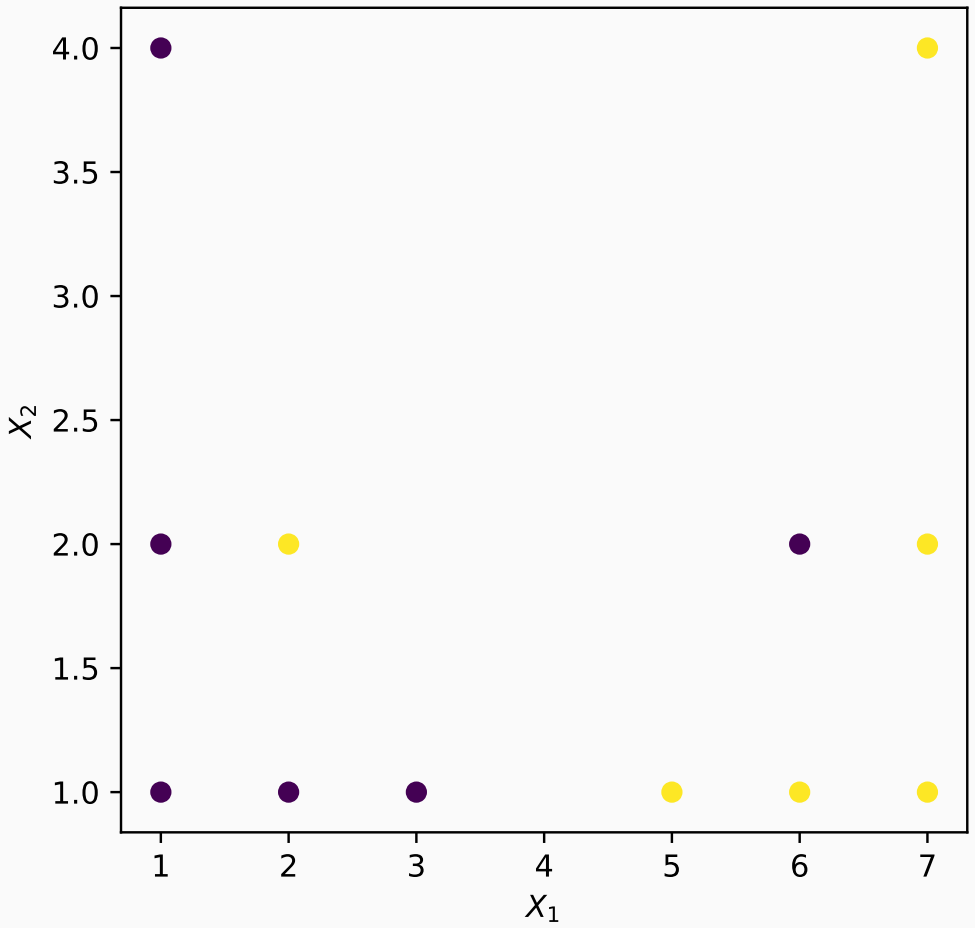
Nipun Batra and teaching staff

July 21, 2025

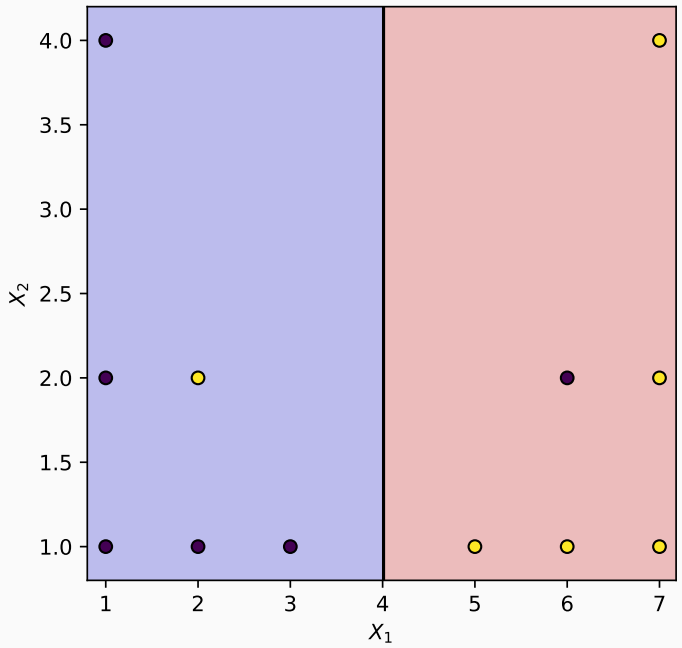
IIT Gandhinagar

A Question!

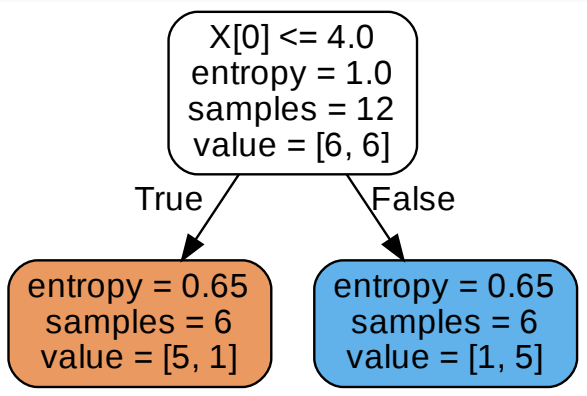
What would be the decision boundary of a decision tree classifier?



Decision Boundary for a tree with depth 1

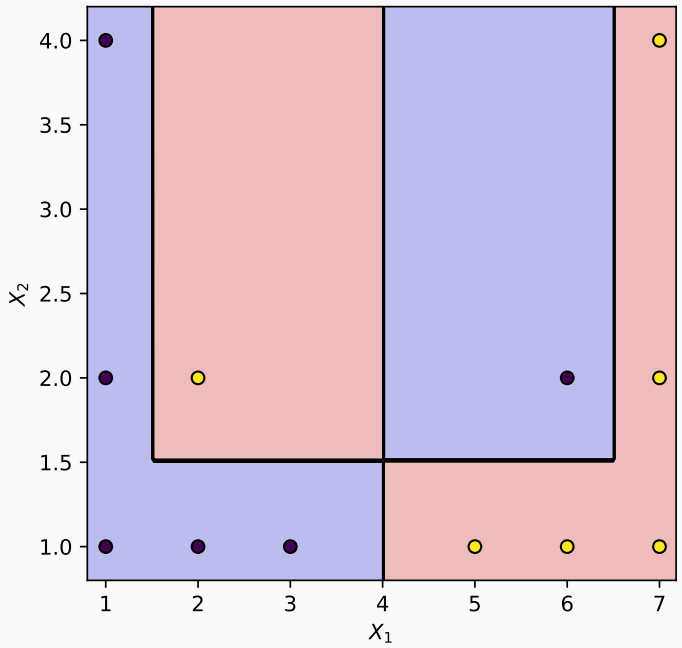


Decision Boundary

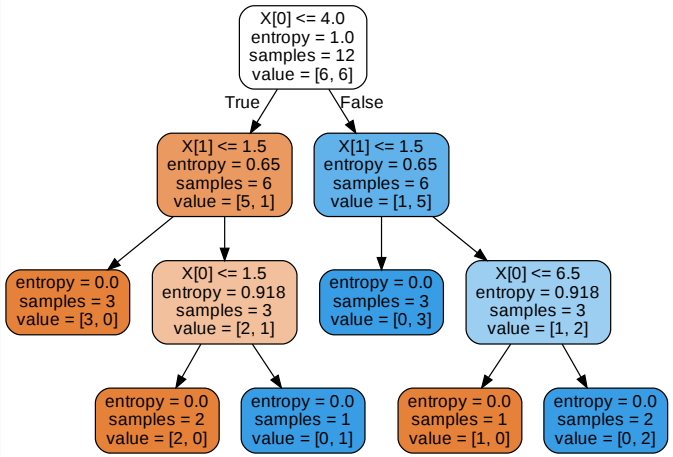


Decision Tree

Decision Boundary for a tree with no depth limit



Decision Boundary



Decision Tree

Are deeper trees always better?

As we saw, deeper trees learn more complex decision boundaries.

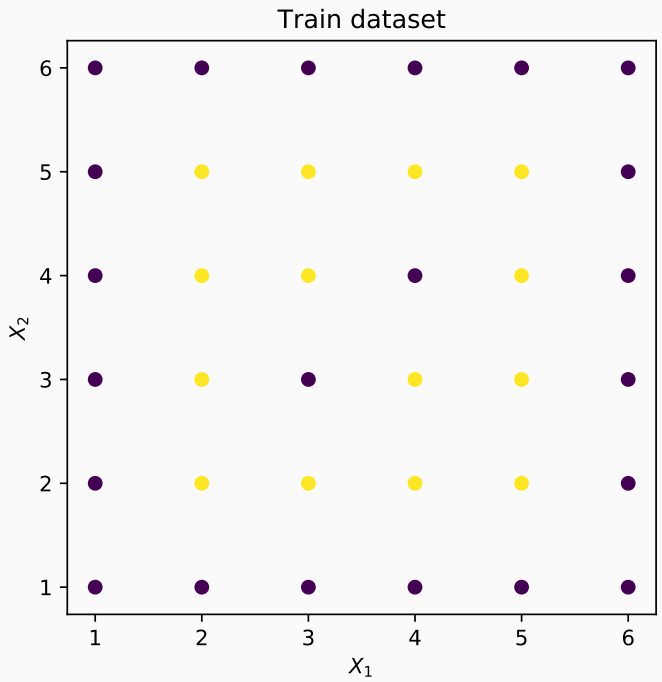
Are deeper trees always better?

As we saw, deeper trees learn more complex decision boundaries.

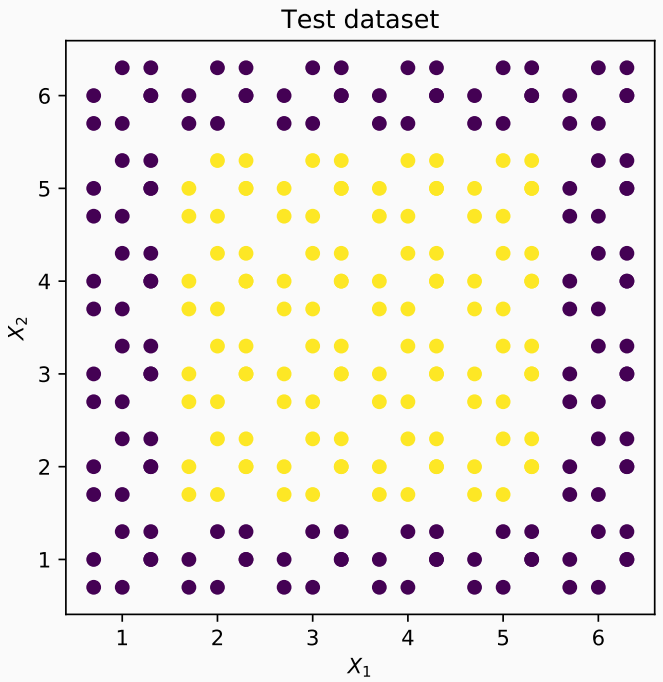
But, sometimes this can lead to poor generalization

An example

Consider the dataset below



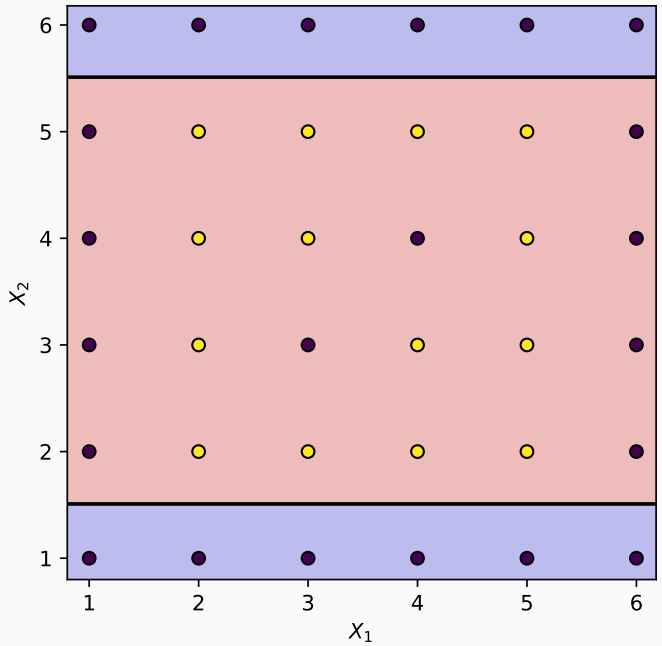
Train Set



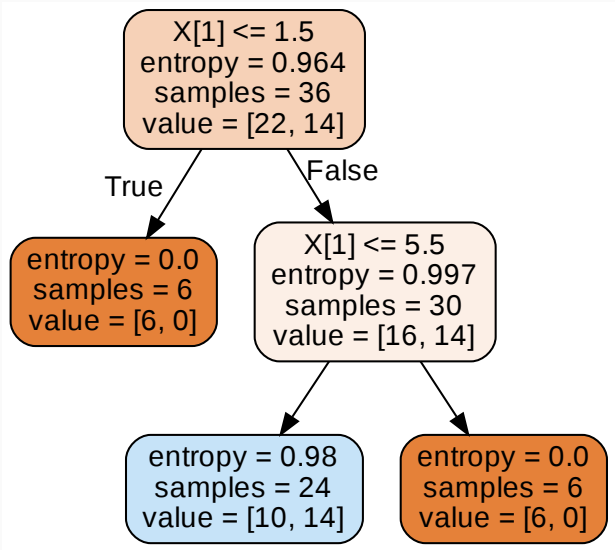
Test Set

Underfitting

Underfitting is also known as high bias, since it has a very biased incorrect assumption.



Decision Boundary

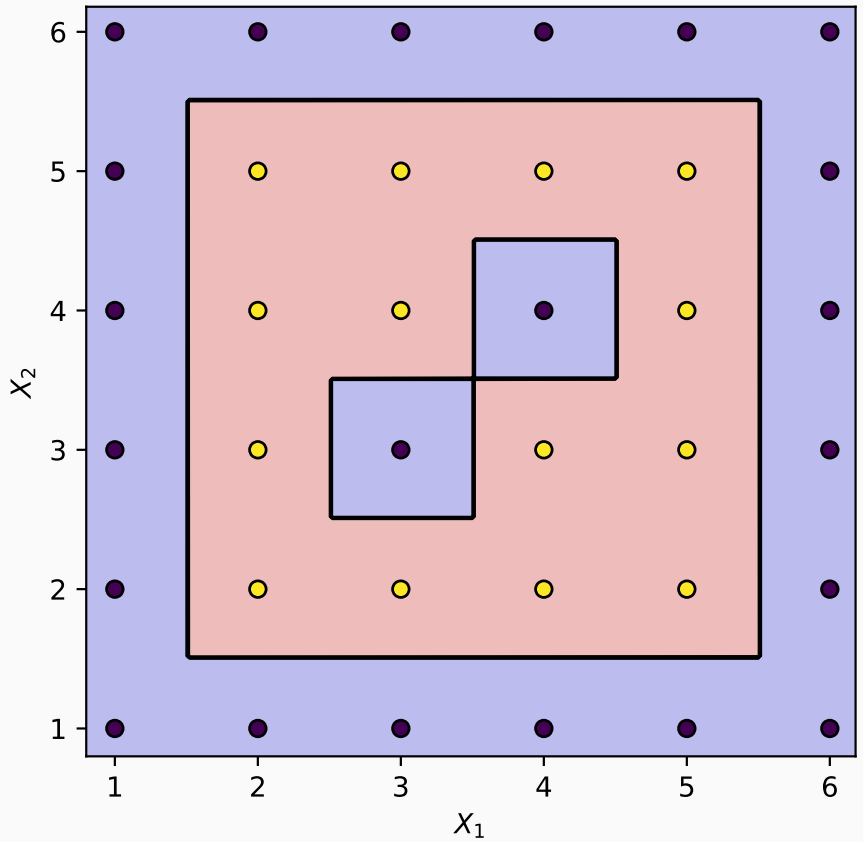


Decision Tree

Overfitting

Overfitting is also known as high variance, since very small changes in data can lead to very different models.

Decision tree learned has depth of 10.



Intuition for Variance

A small change in data can lead to very different models.

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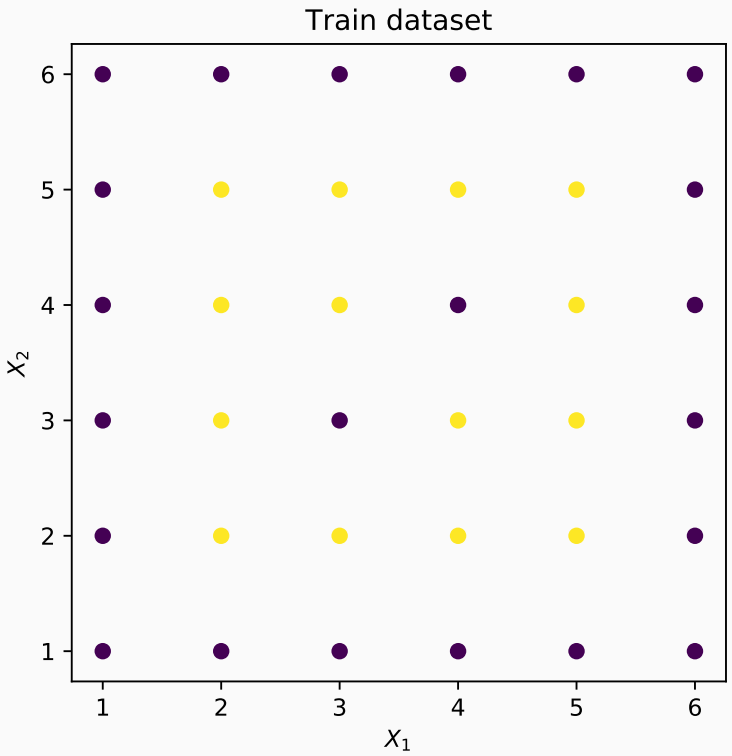
Dataset 1



Intuition for Variance

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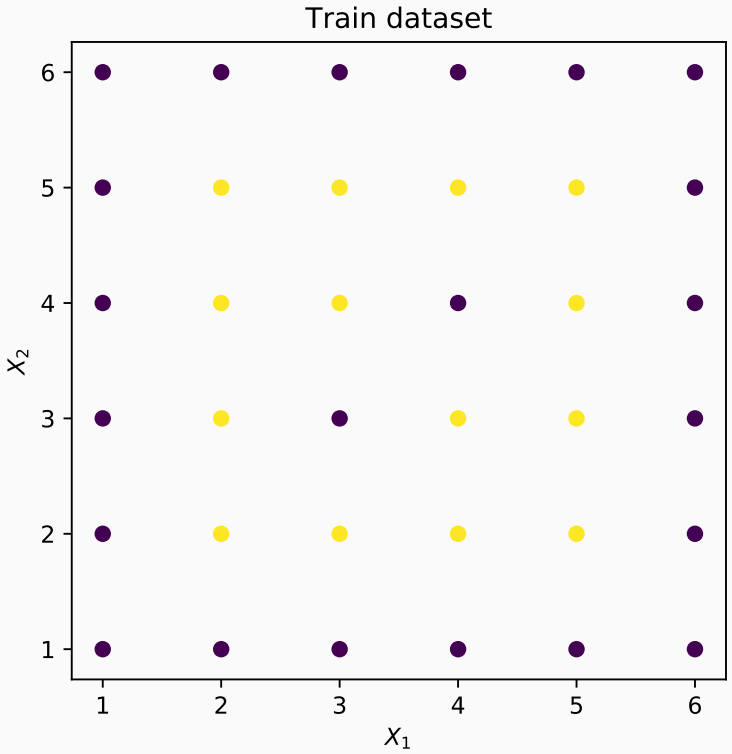
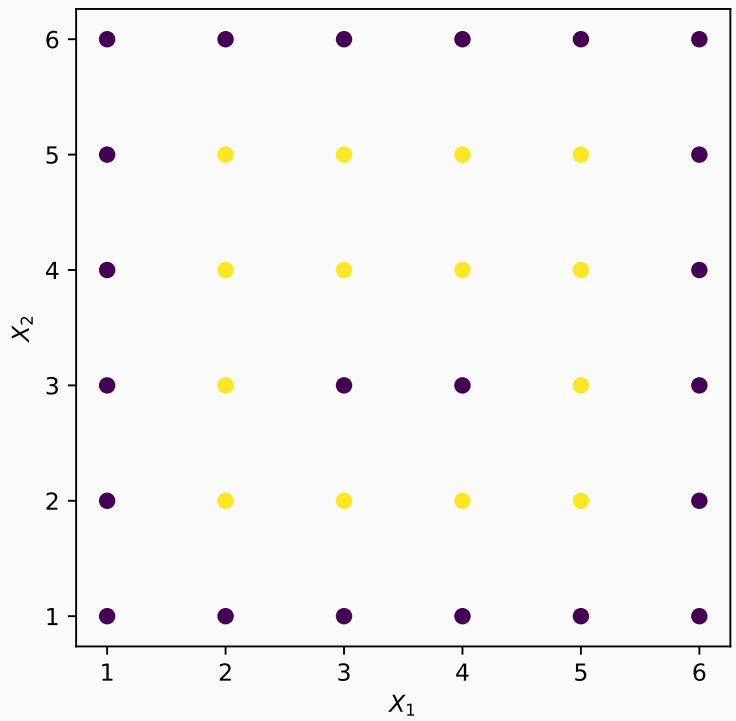
Dataset 1



Dataset 2



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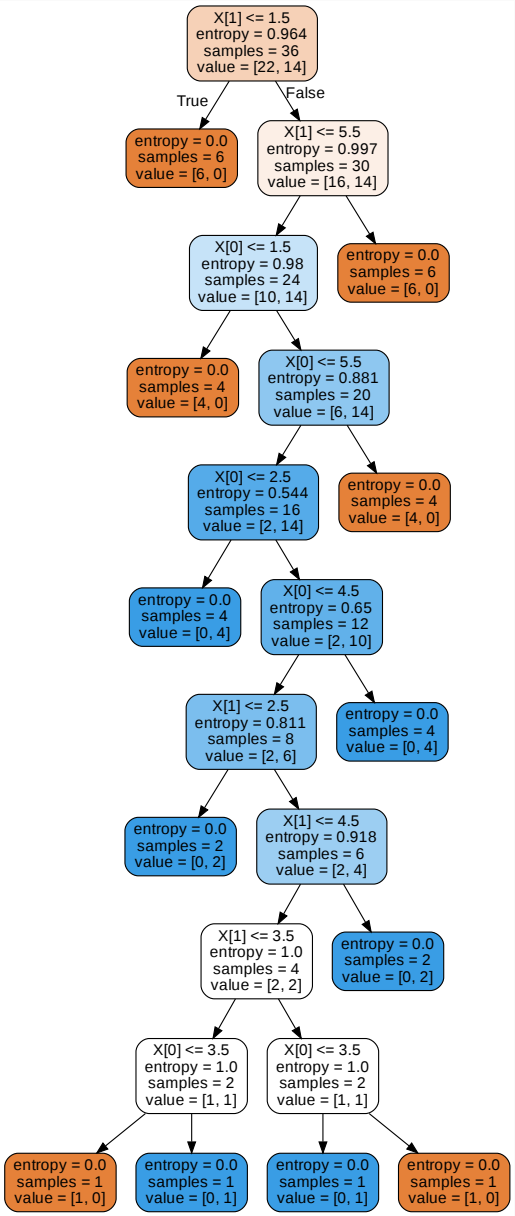
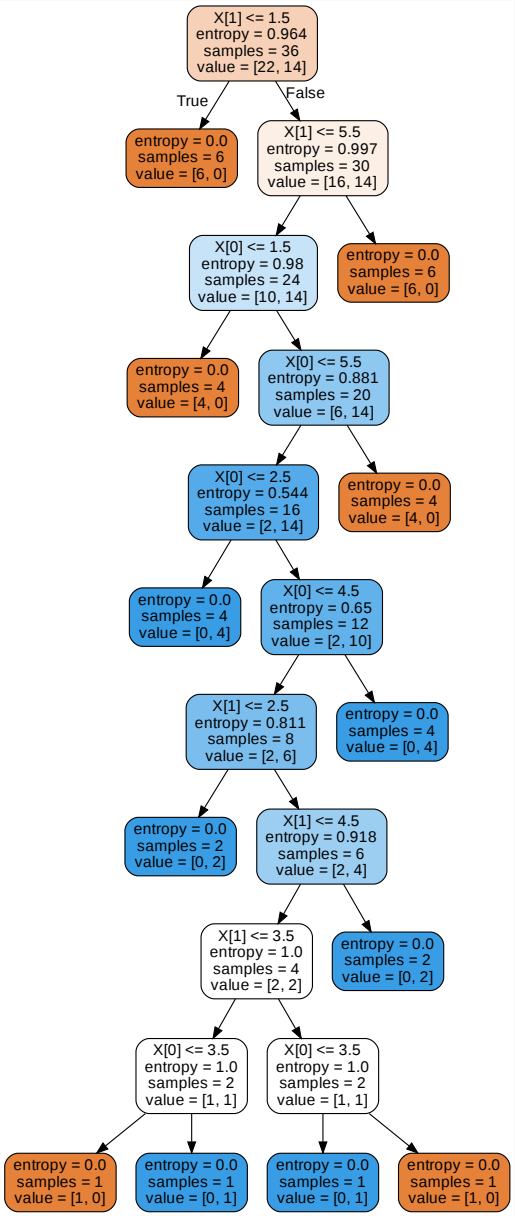
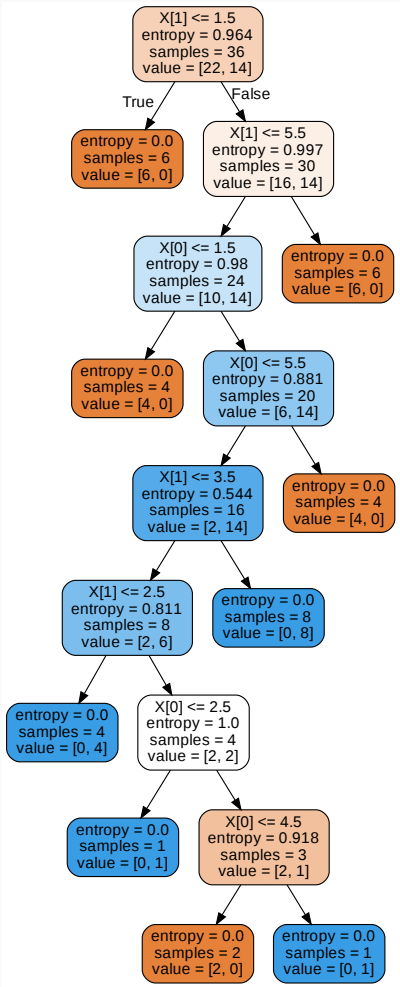


Intuition for Variance





A Good Fit

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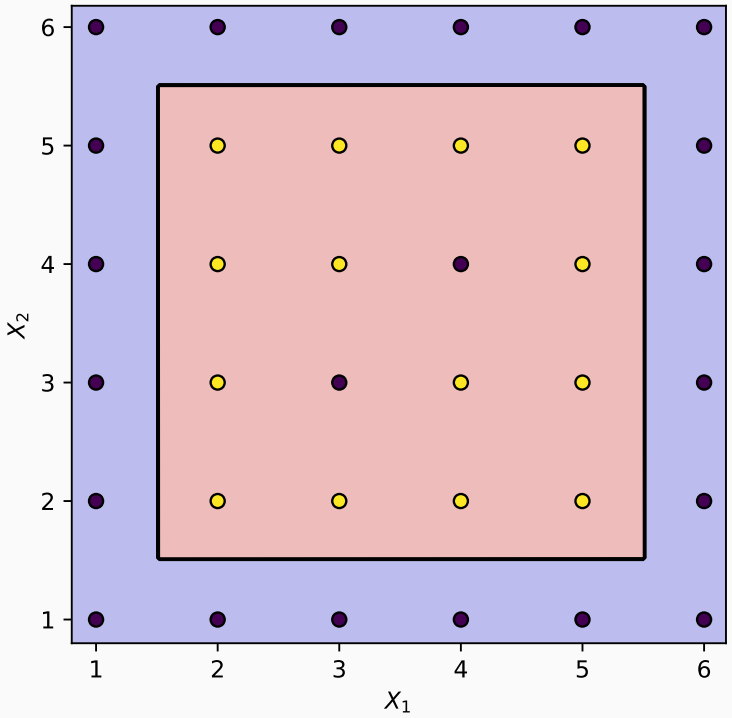

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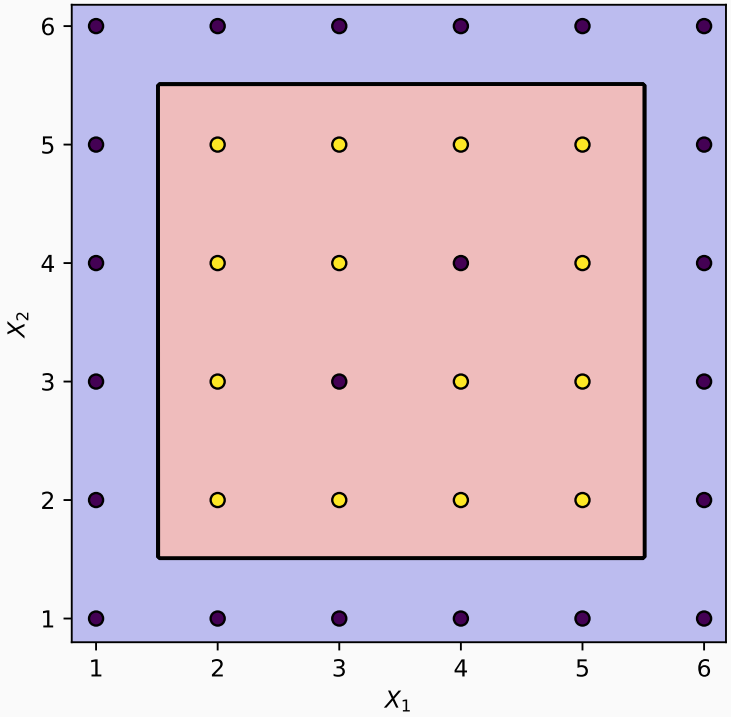
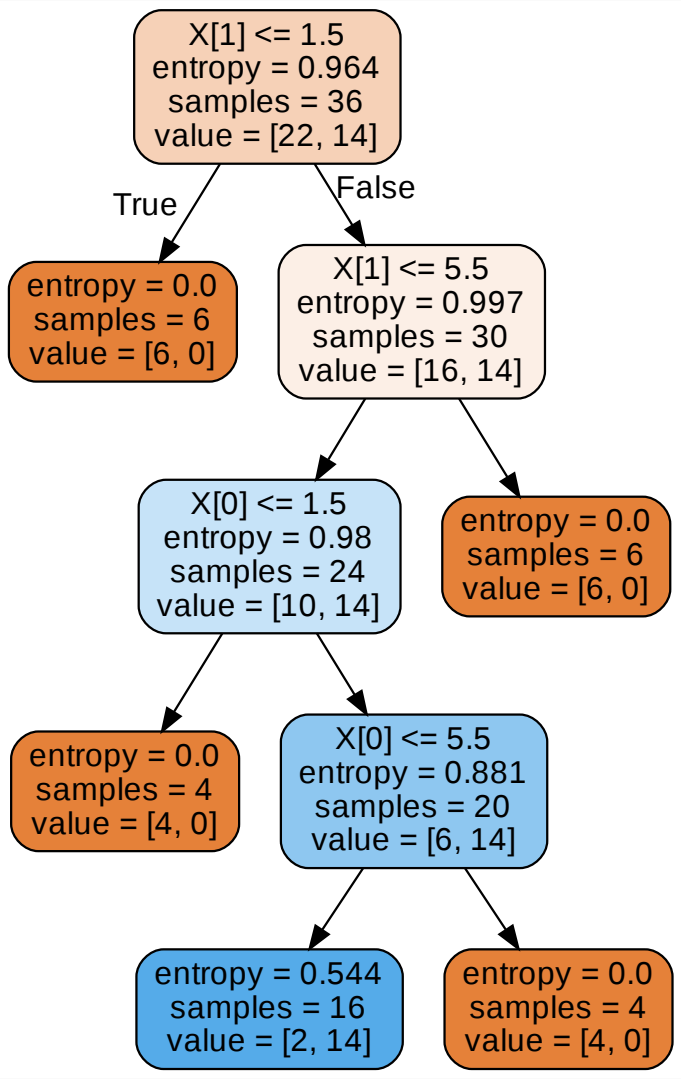
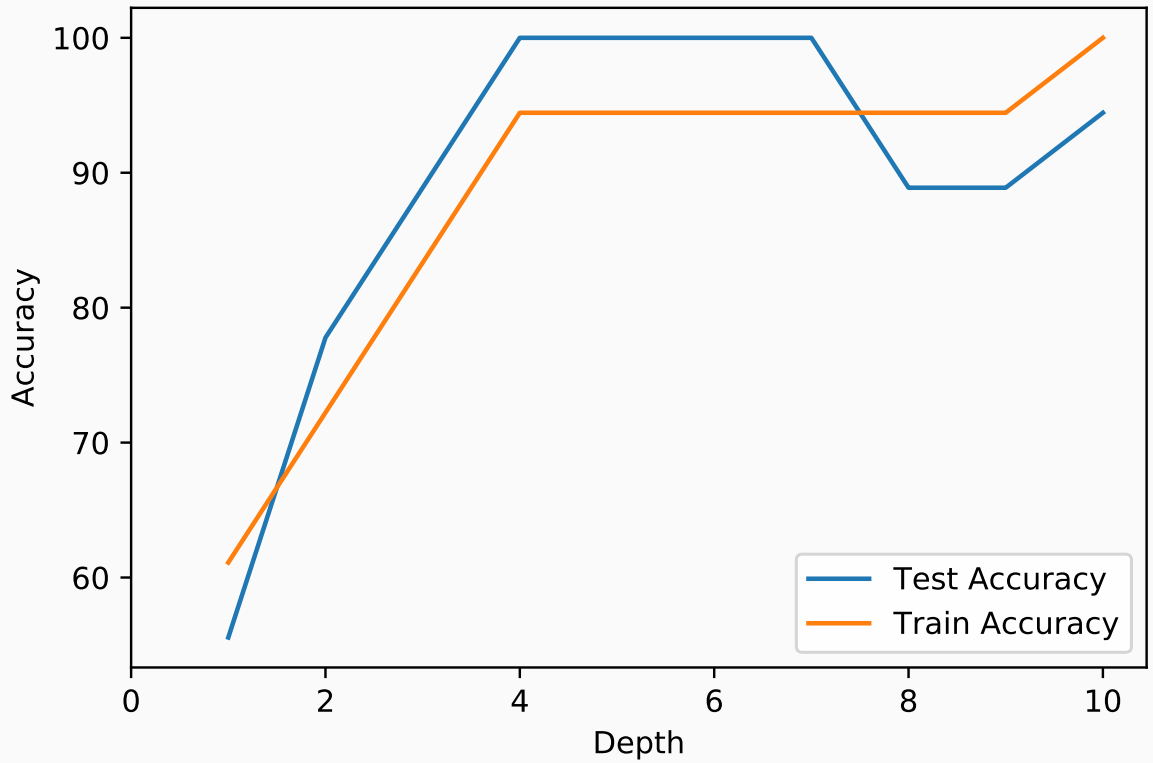
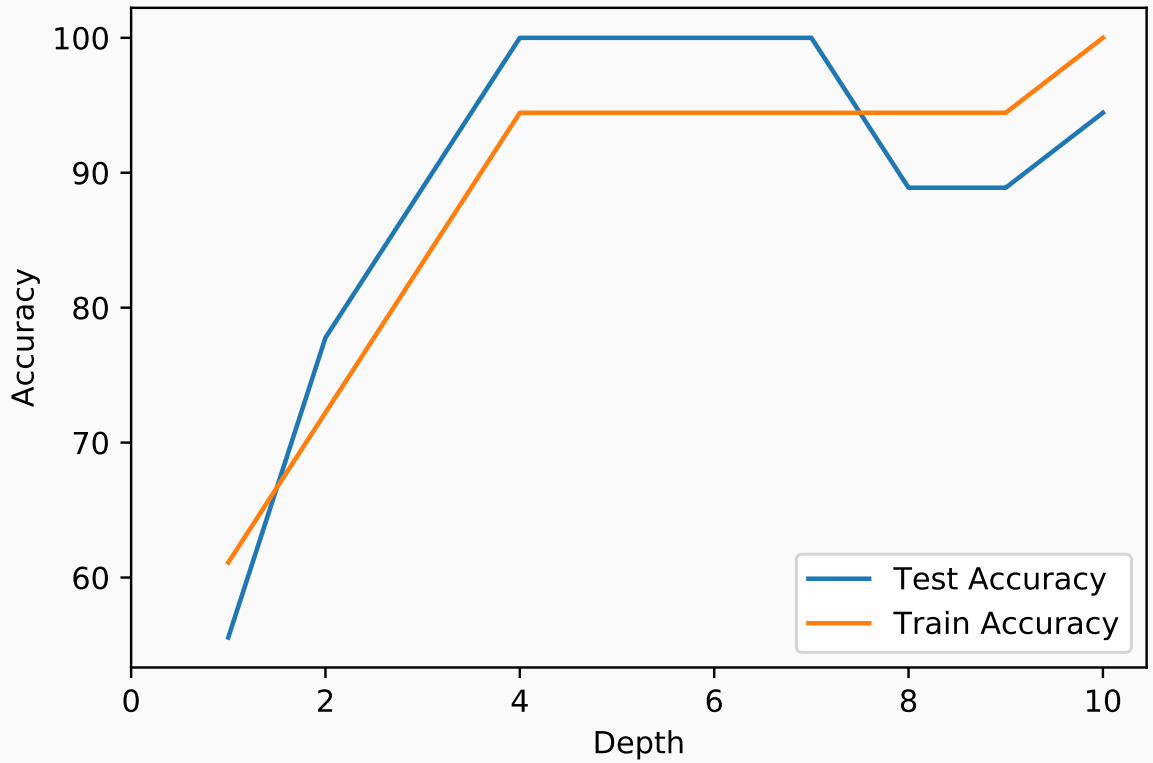

6
5
4
3
2
1
X_2
1
2
3
4
5
6
X_1


X[1] <= 1.5
entropy = 0.964
samples = 36
value = [22, 14]
True
False
entropy = 0.0
samples = 6
value = [6, 0]
X[1] <= 5.5
entropy = 0.997
samples = 30
value = [16, 14]
X[0] <= 1.5
entropy = 0.98
samples = 24
value = [10, 14]
entropy = 0.0
samples = 6
value = [6, 0]
entropy = 0.0
samples = 4
value = [4, 0]
X[0] <= 5.5
entropy = 0.881
samples = 20
value = [6, 14]
entropy = 0.544
samples = 16
value = [2, 14]
entropy = 0.0
samples = 4
value = [4, 0]

Accuracy vs Depth Curve

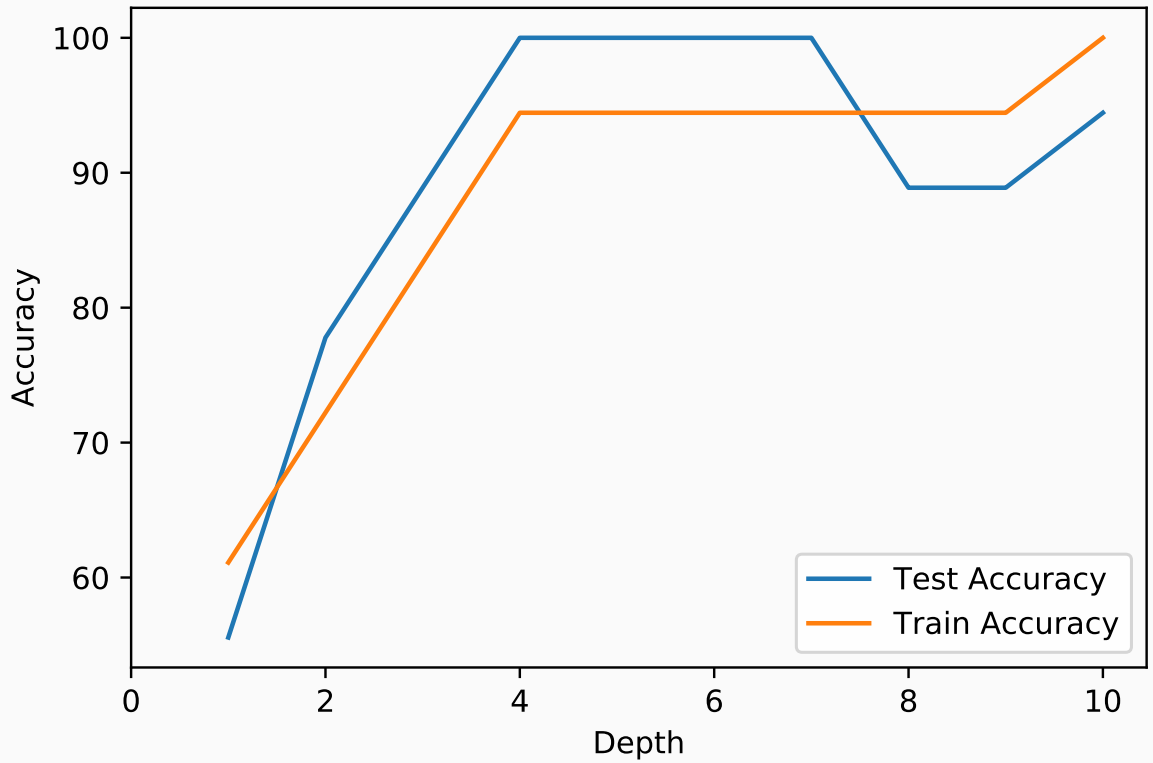


Accuracy vs Depth Curve



As depth increases, train accuracy improves

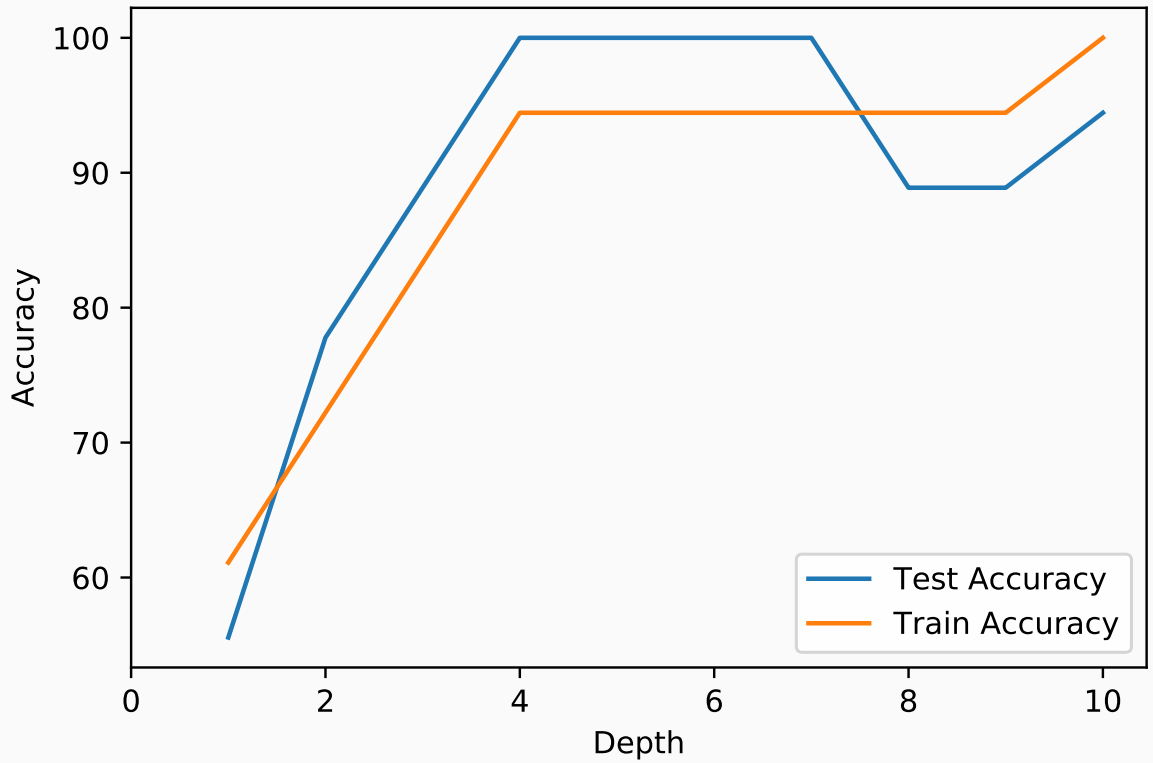
Accuracy vs Depth Curve



As depth increases, train accuracy improves

As depth increases, test accuracy improves till a point

Accuracy vs Depth Curve



As depth increases, train accuracy improves

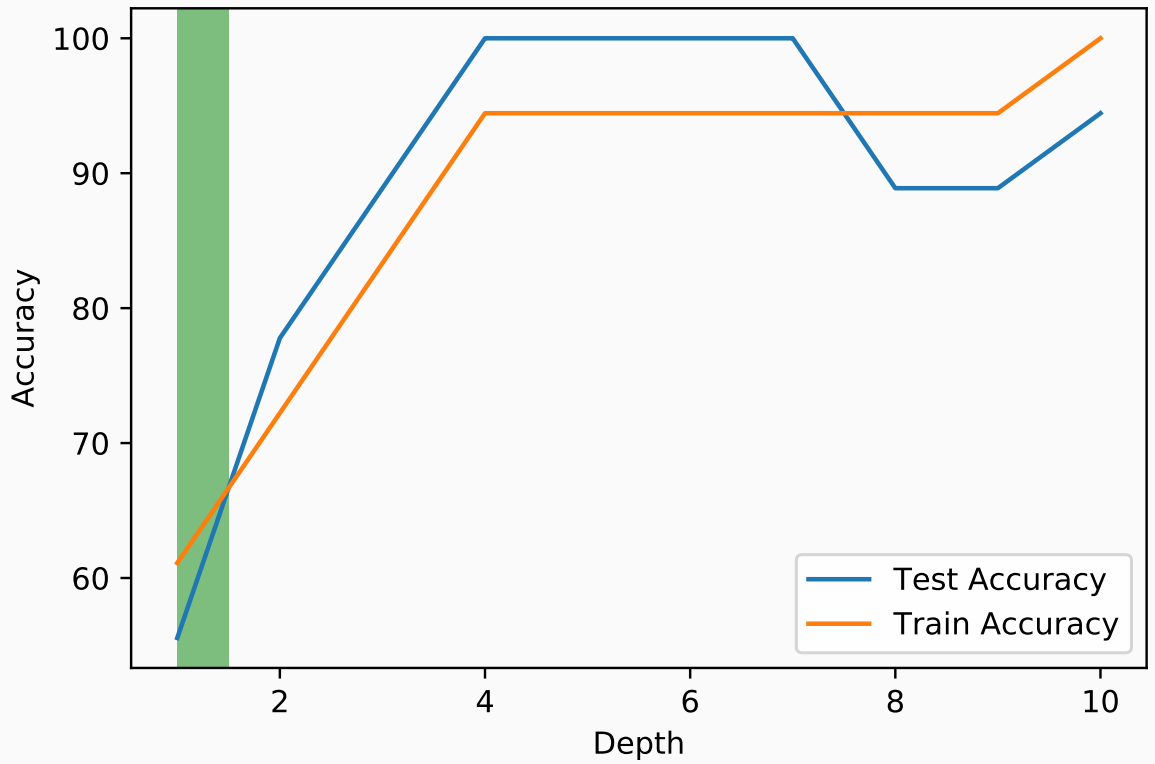
As depth increases, test accuracy improves till a point

At very high depths, test accuracy is not good (overfitting).

Accuracy vs Depth Curve : Underfitting

The highlighted region is the underfitting region.

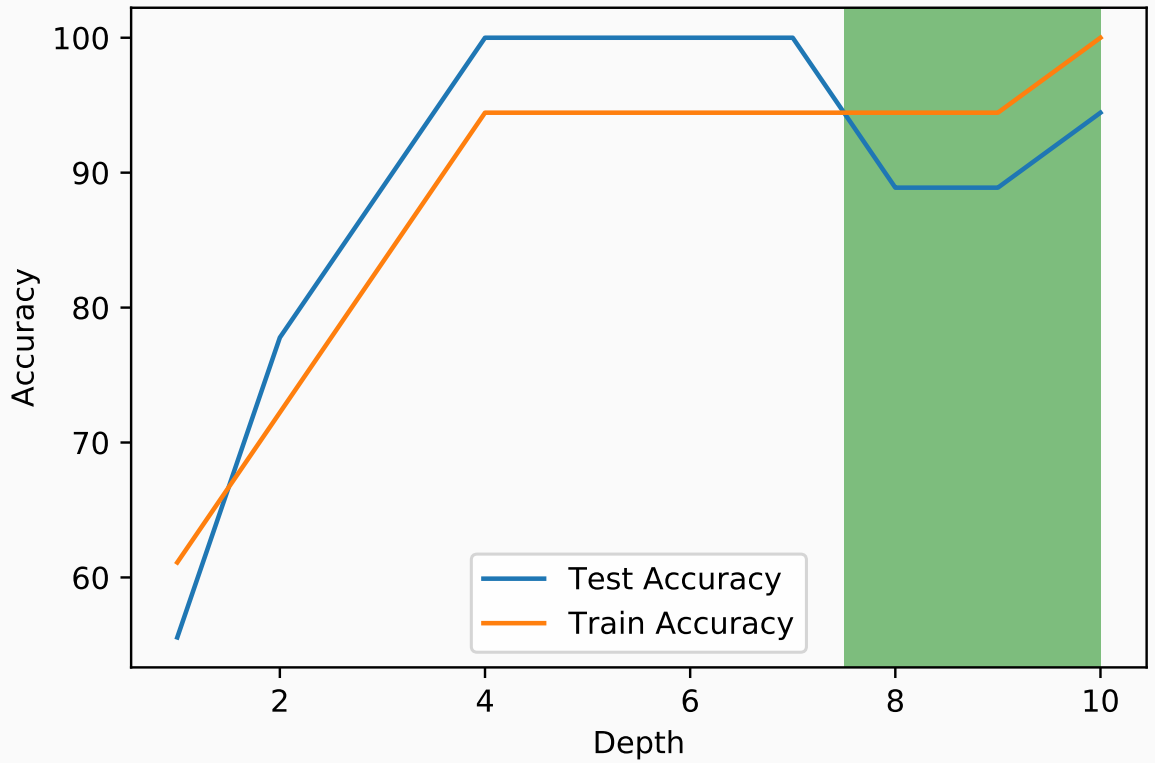
Model is too simple (less depth) to learn from the data.



Accuracy vs Depth Curve : Overfitting

The highlighted region is the overfitting region.

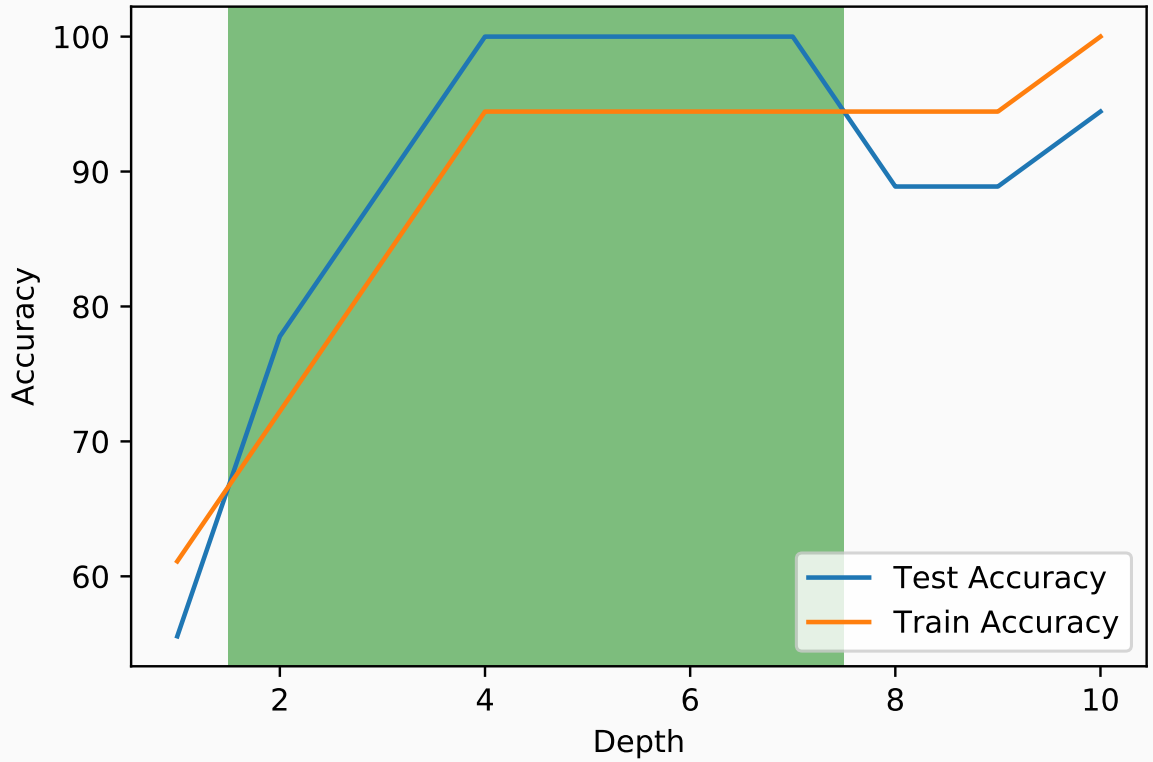
Model is complex (high depth) and hence also learns the anomalies in data.



Accuracy vs Depth Curve

The highlighted region is the good fit region.

We want to maximize test accuracy while being in this region.



The big question!?

How to find the optimal depth for a decision tree?

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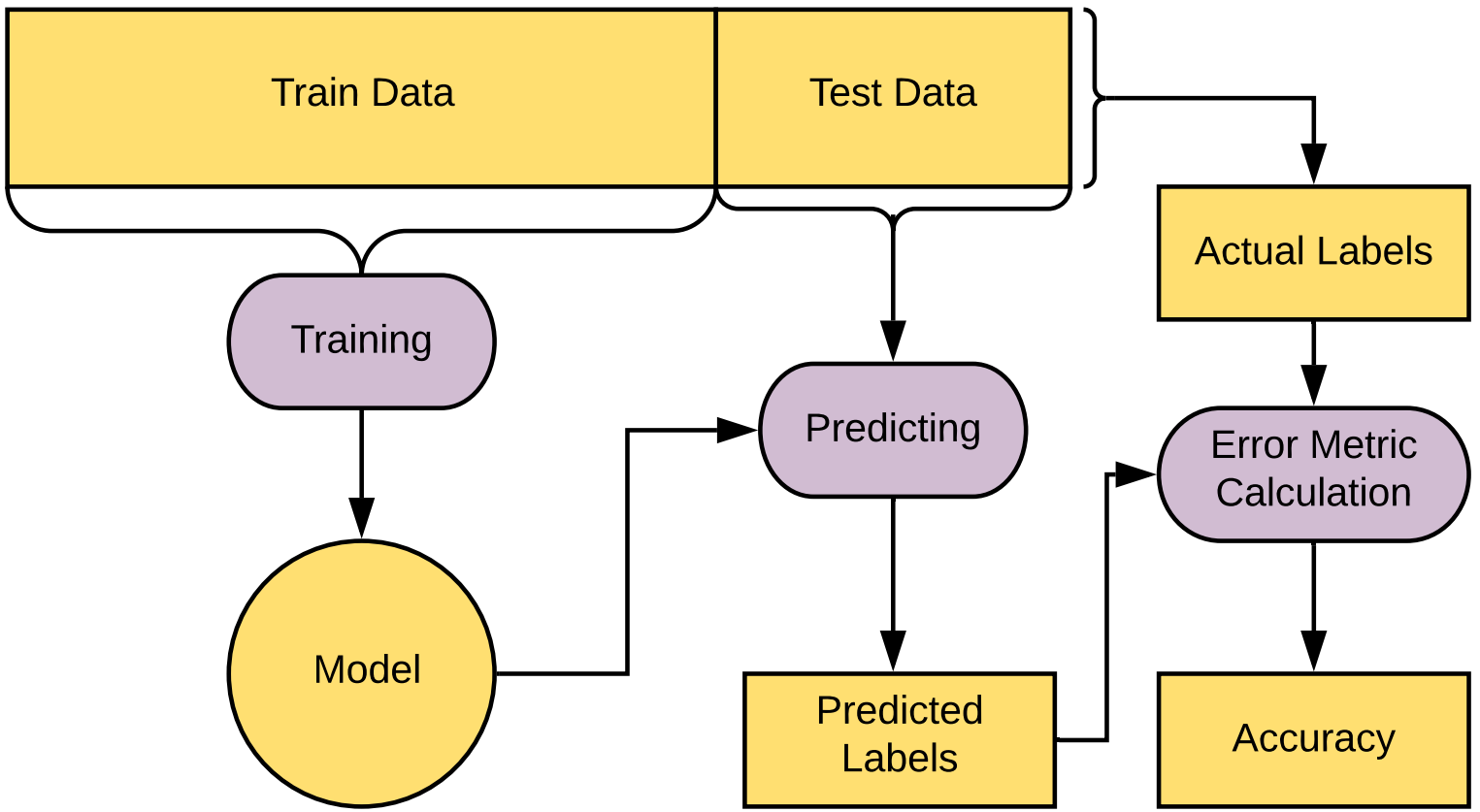
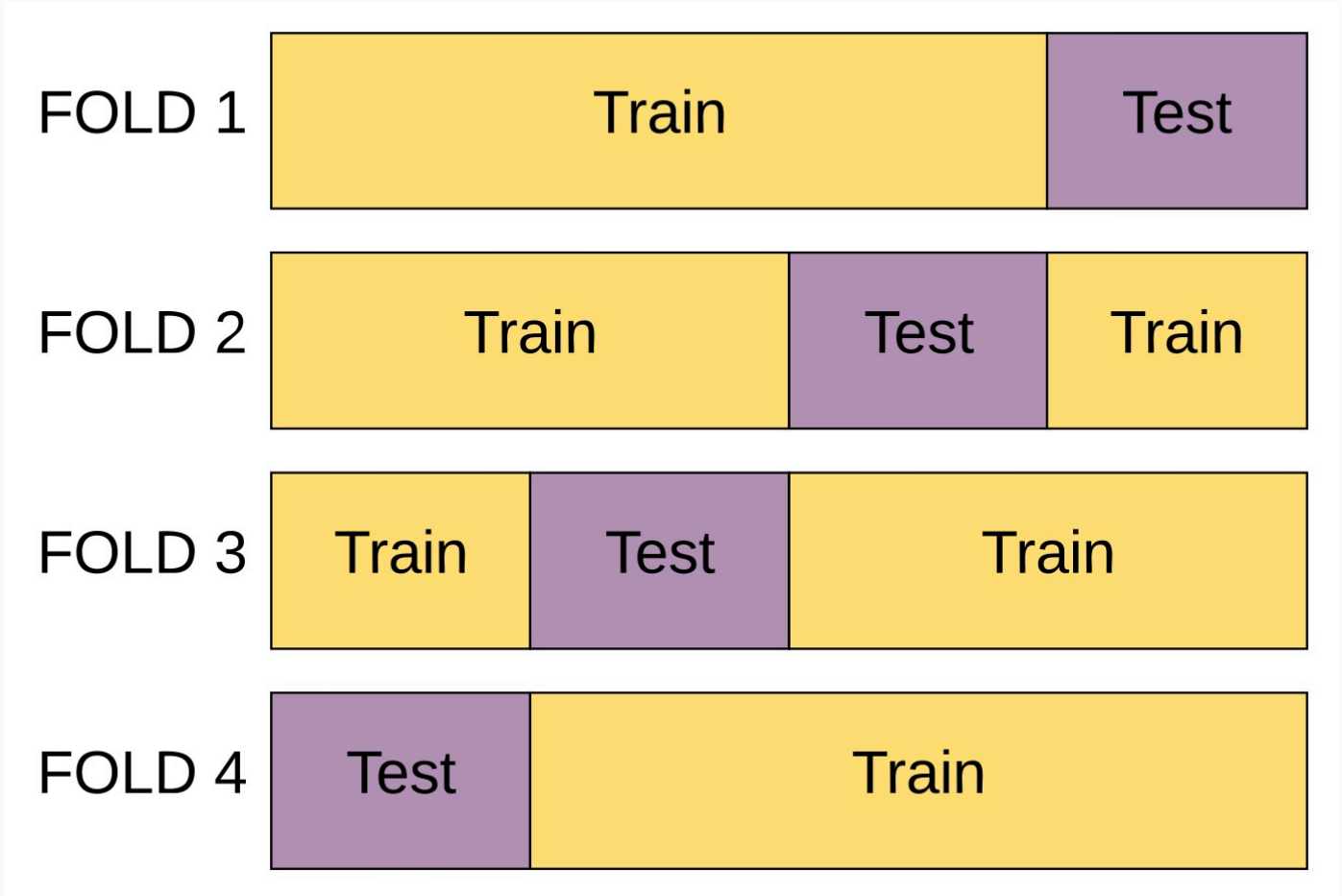
Use cross-validation!

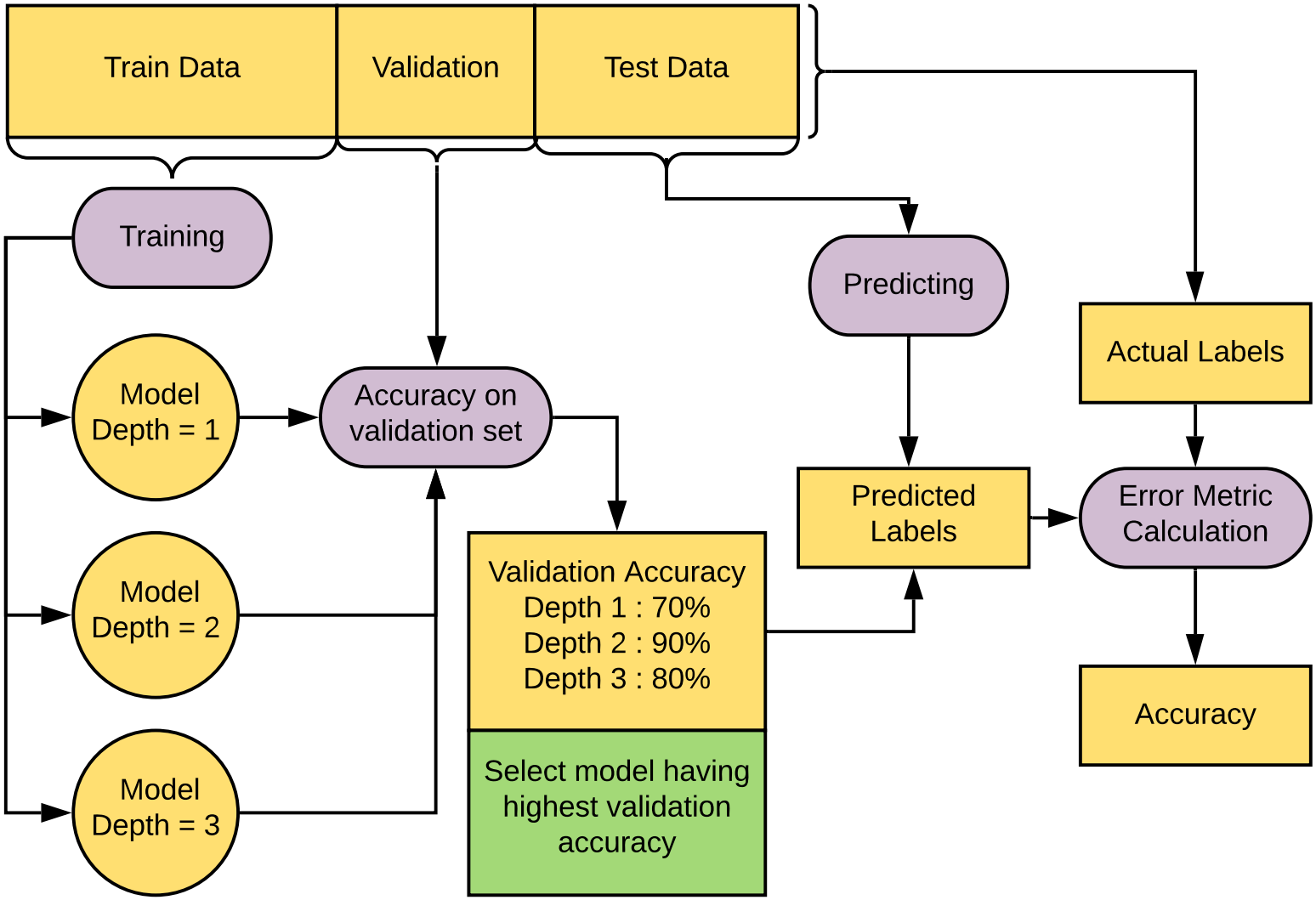
Our General Training Flow



K-Fold cross-validation: Utilise full dataset for testing



The Validation Set

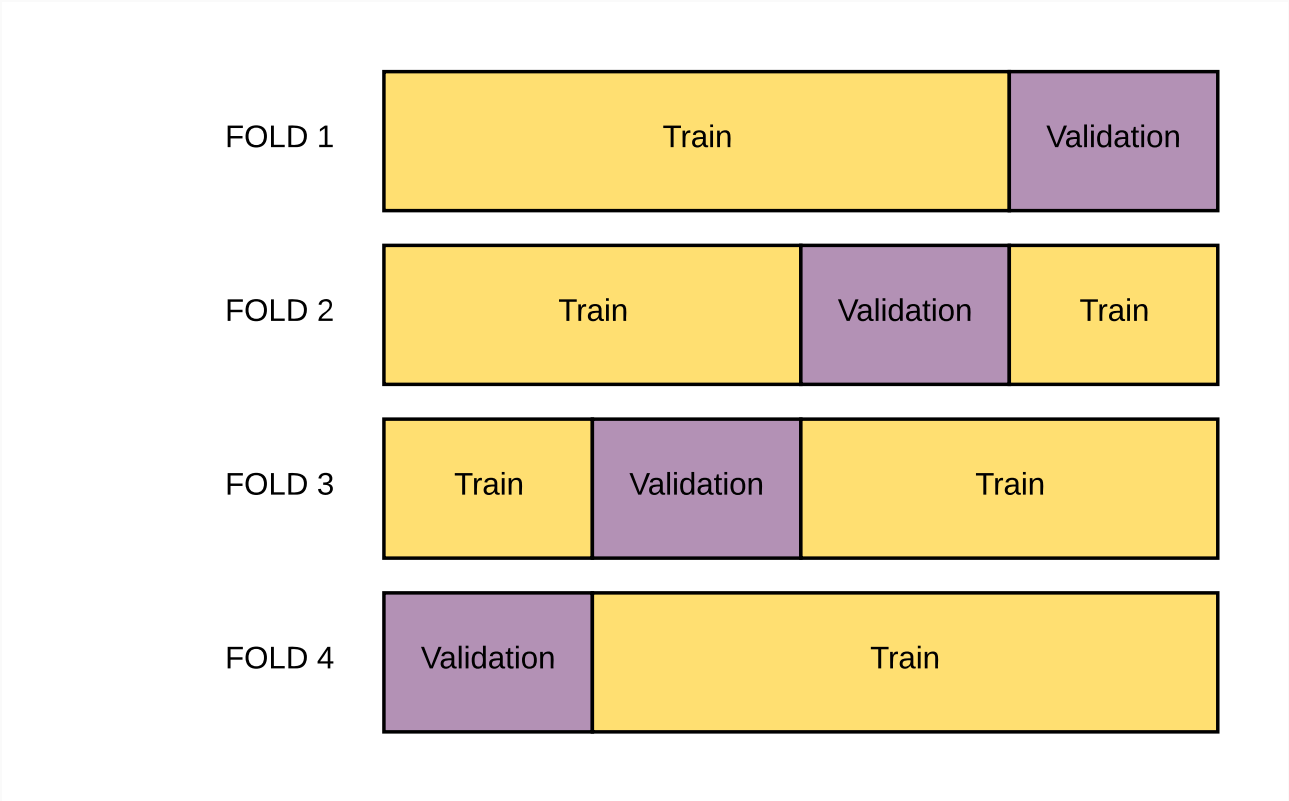


Nested Cross Validation

Divide your training set into k equal parts.

Cyclically use 1 part as "validation set" and the rest for training.

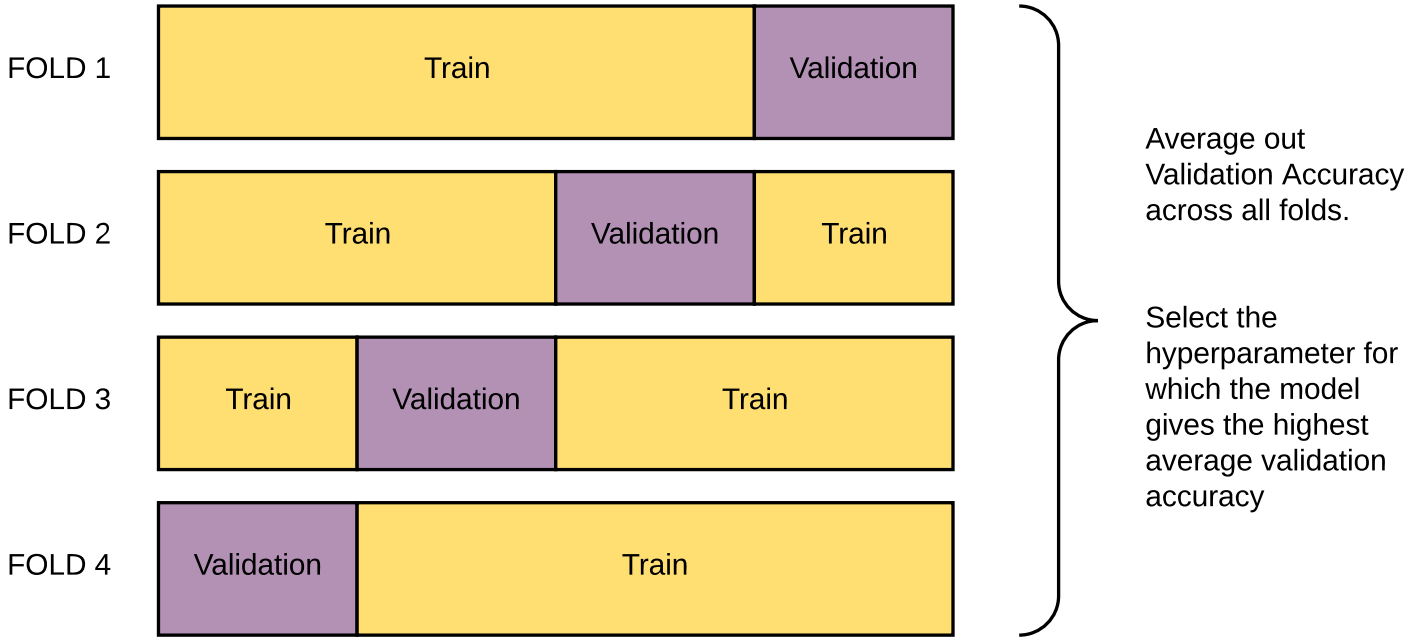
Here $k = 4$



Nested Cross Validation

Average out the validation accuracy across all the folds

Use the model with highest validation accuracy



Next time: Ensemble Learning

- How to combine various models?

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- Why to combine multiple models?

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- How to combine various models?
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- How can we reduce bias?
- How can we reduce variance?